

10/049,823

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Apr 08	"Ask CAS" for self-help around the clock
NEWS	3	Jun 03	New e-mail delivery for search results now available
NEWS	4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS	5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS	6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS	7	Sep 03	JAPIO has been reloaded and enhanced
NEWS	8	Sep 16	Experimental properties added to the REGISTRY file
NEWS	9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS	10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS	11	Oct 24	BEILSTEIN adds new search fields
NEWS	12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS	13	Nov 18	DKILIT has been renamed APOLLIT
NEWS	14	Nov 25	More calculated properties added to REGISTRY
NEWS	15	Dec 04	CSA files on STN
NEWS	16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS	17	Dec 17	TOXCENTER enhanced with additional content
NEWS	18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS	19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS	20	Feb 13	CANCERLIT is no longer being updated
NEWS	21	Feb 24	METADEX enhancements
NEWS	22	Feb 24	PCTGEN now available on STN
NEWS	23	Feb 24	TEMA now available on STN
NEWS	24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS	25	Feb 26	PCTFULL now contains images
NEWS	26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS	27	Mar 20	EVENTLINE will be removed from STN
NEWS	28	Mar 24	PATDPAFULL now available on STN
NEWS	29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS	30	Apr 11	Display formats in DGENE enhanced
NEWS	31	Apr 14	MEDLINE Reload
NEWS	32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS	33	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS	34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS	35	Apr 28	RDISCLOSURE now available on STN
NEWS	36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS	37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS	38	May 15	Supporter information for ENCOMPAT and ENCOMPLIT updated
NEWS	39	May 16	CHEMREACT will be removed from STN
NEWS	40	May 19	Simultaneous left and right truncation added to WSCA
NEWS	41	May 19	RAPRA enhanced with new search field, simultaneous left and

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right truncation

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
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FILE 'HOME' ENTERED AT 14:17:53 ON 23 MAY 2003

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:18:02 ON 23 MAY 2003

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STRUCTURE FILE UPDATES: 22 MAY 2003 HIGHEST RN 519137-84-9

DICTIONARY FILE UPDATES: 22 MAY 2003 HIGHEST RN 519137-84-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when  
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading 10049823.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 14:18:20 FILE 'REGISTRY'

10/049,823

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2 TO 124  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful  
FULL SEARCH INITIATED 14:18:33 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 46 TO ITERATE

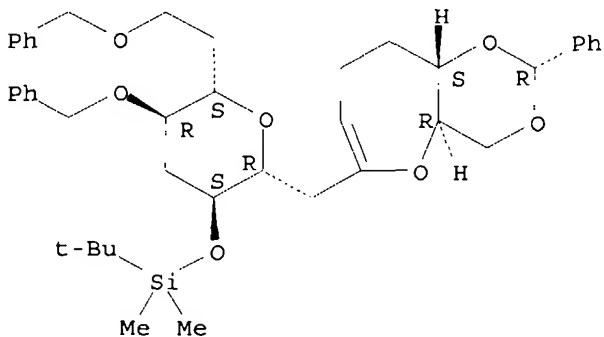
100.0% PROCESSED 46 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> d scan

L3 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Silane, (1,1-dimethylethyl)dimethyl[[[(2R,3S,5R,6S)-tetrahydro-5-(phenylmethoxy)-6-[2-(phenylmethoxy)ethyl]-2-[[[(2R,4aR,9aS)-4a,8,9,9a-tetrahydro-2-phenyl-4H-1,3-dioxino[5,4-b]oxepin-6-yl]methyl]-2H-pyran-3-yl]oxy]- (9CI)  
MF C42 H56 O7 Si

Absolute stereochemistry. Rotation (+).



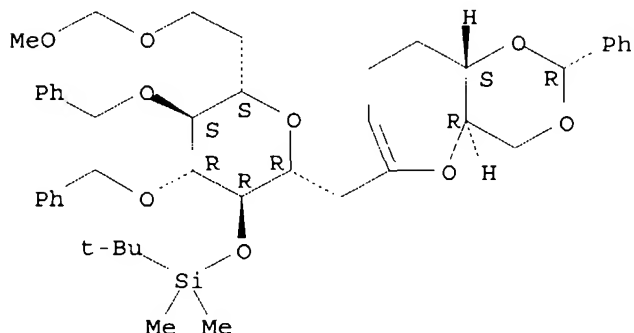
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN L-arabino-L-allo-Pentadec-6-enitol, 2,7:9,13-dianhydro-4,5,6,8,14-pentadeoxy-10-O-[(1,1-dimethylethyl)dimethylsilyl]-15-O-(methoxymethyl)-11,12-bis-O-(phenylmethyl)-1,3-O-[(R)-phenylmethylene]- (9CI)  
MF C44 H60 O9 Si

10/049,823

Absolute stereochemistry. Rotation (+).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.15

148.36

FILE 'CAPLUS' ENTERED AT 14:18:52 ON 23 MAY 2003

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FILE COVERS 1907 - 23 May 2003 VOL 138 ISS 22

FILE LAST UPDATED: 22 May 2003 (20030522/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 and (prepar? or synthes? or make or made or process)

6 L3

1401752 PREPAR?

105014 PREP

1884 PREPS

106706 PREP

(PREP OR PREPS)

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1802532 PREPD  
21 PREPDS  
1802547 PREPD  
(PREPD OR PREPDS)  
89007 PREPG  
12 PREPGS  
89018 PREPG  
(PREPG OR PREPGS)  
2309463 PREPN  
183748 PREPNS  
2450448 PREPN  
(PREPN OR PREPNS)  
4132690 PREPAR?  
(PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)  
1291701 SYNTHES?  
173342 MAKE  
129462 MAKES  
295471 MAKE  
(MAKE OR MAKES)  
1049766 MADE  
22 MADES  
1049785 MADE  
(MADE OR MADES)  
1806803 PROCESS  
1172688 PROCESSES  
2670629 PROCESS  
(PROCESS OR PROCESSES)  
L4 6 L3 AND (PREPAR? OR SYNTHES? OR MAKE OR MADE OR PROCESS)

=> s l4 and catalyst  
625179 CATALYST  
625065 CATALYSTS  
800032 CATALYST  
(CATALYST OR CATALYSTS)

L5 4 L4 AND CATALYST

=> d l4 ibib hitstr abs 1-6

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS  
ACCESSION NUMBER: 2002:150043 CAPLUS  
DOCUMENT NUMBER: 137:93629  
TITLE: A general strategy for the convergent  
**synthesis** of fused polycyclic ethers via  
B-alkyl Suzuki coupling: **synthesis** of the  
ABCD ring fragment of ciguatoxins  
AUTHOR(S): Sasaki, Makoto; Ishikawa, Makoto; Fuwa, Haruhiko;  
Tachibana, Kazuo  
CORPORATE SOURCE: Graduate School of Science, Department of Chemistry,  
The University of Tokyo, and CREST, Japan Science and  
Technology Corporation (JST), Hongo, Bunkyo-ku, Tokyo,  
113-0033, Japan  
SOURCE: Tetrahedron (2002), 58(10), 1889-1911  
CODEN: TETRAB; ISSN: 0040-4020  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 137:93629  
IT 250226-82-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)

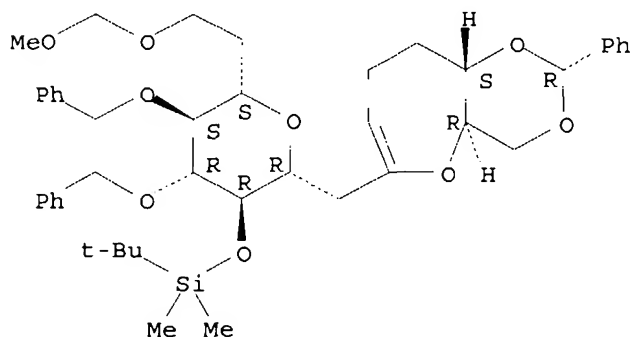
10/049,823

(**synthesis** of the ABCD ring subunit of ciguatoxins via convergent **synthesis** of fused polycyclic ethers using B-alkyl Suzuki coupling)

RN 250226-82-5 CAPLUS

CN L-arabino-L-allo-Pentadec-6-enitol, 2,7:9,13-dianhydro-4,5,6,8,14-pentadeoxy-10-O-[(1,1-dimethylethyl)dimethylsilyl]-15-O-(methoxymethyl)-11,12-bis-O-(phenylmethyl)-1,3-O-[(R)-phenylmethylene]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB A new method for convergent coupling of fused polycyclic ethers has been developed, which relies on B-alkyl Suzuki cross-coupling of lactone-derived enol triflates or phosphates. The strategy was successfully applied to a convergent **synthesis** of the ABCD ring fragment 4 of ciguatoxins, the causative toxin for ciguatera fish poisoning. The synthetic route includes a convergent union of the B and D rings by the B-alkyl Suzuki coupling, introduction of a double bond into the D ring followed by reductive closure of the tetrahydropyran C ring to afford the BCD ring system, and, finally, ring-closing metathesis reaction to construct the oxepene A ring.

REFERENCE COUNT: 150 THERE ARE 150 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:935611 CAPLUS

DOCUMENT NUMBER: 136:53638

TITLE: **Process** for preparing cyclic polyethers

INVENTOR(S): Sasaki, Makoto; Tachibana, Kazuo; Fuwa, Haruhiko

PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan

SOURCE: PCT Int. Appl., 18 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

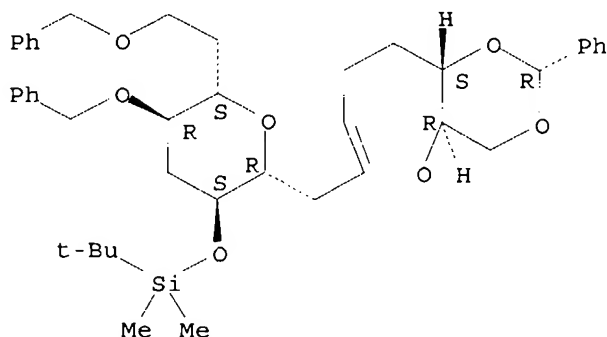
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098308	A1	20011227	WO 2001-JP1872	20010309
W: CA, US				
JP 2002003494	A2	20020109	JP 2000-182148	20000616

10/049,823

PRIORITY APPLN. INFO.: JP 2000-182148 A 20000616  
OTHER SOURCE(S): CASREACT 136:53638  
IT 315203-88-4P  
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(**process** for **prepg.** cyclic polyethers)  
RN 315203-88-4 CAPLUS  
CN Silane, (1,1-dimethylethyl)dimethyl[[(2R,3S,5R,6S)-tetrahydro-5-(phenylmethoxy)-6-[2-(phenylmethoxy)ethyl]-2-[[[(2R,4aR,9aS)-4a,8,9,9a-tetrahydro-2-phenyl-4H-1,3-dioxino[5,4-b]oxepin-6-yl]methyl]-2H-pyran-3-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB This document discloses a **process** for **synthesizing** cyclic polyether skeletons convergently without using an excess of a phosphate at room temp. in high yield, which **process** is applicable to the **synthesis** of gambierol and ciguatoxin. This **process** comprises cross-coupling an alkylborane with a cyclic ketene acetal phosphate in the presence of an aq. basic soln. by using chloro[1,1'-bis(diphenylphosphino)ferrocene]palladium as the catalyst.  
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:531967 CAPLUS

DOCUMENT NUMBER: 135:122407

TITLE: **Preparation** of (large-membered) cyclic polyethers from alkylboranes and cyclic enol phosphates

INVENTOR(S): Sasaki, Makoto; Fuwa, Haruhiko; Tachibana, Kazuo  
PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.  
CODEN: JKXXAF

DOCUMENT TYPE: Patent  
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001199987	A2	20010724	JP 2000-12277	20000120
PRIORITY APPLN. INFO.:			JP 2000-12277	20000120
OTHER SOURCE(S):		CASREACT 135:122407		

10/049,823

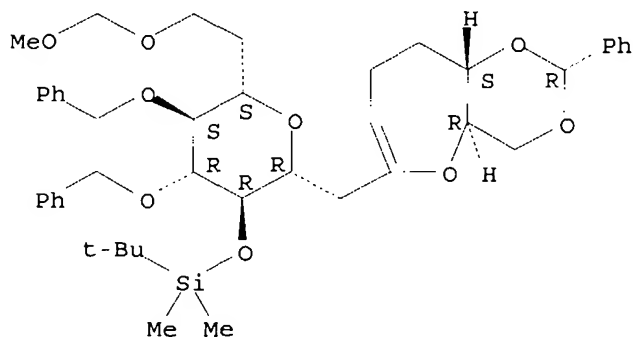
IT 250226-82-5P

RL: IMF (Industrial manufacture); PREP (Preparation)  
(**prepn.** of cyclic polyethers from alkylboranes and cyclic enol phosphates)

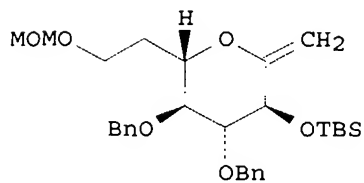
RN 250226-82-5 CAPLUS

CN L-arabino-L-allo-Pentadec-6-enitol, 2,7:9,13-dianhydro-4,5,6,8,14-pentadeoxy-10-O-[(1,1-dimethylethyl)dimethylsilyl]-15-O-(methoxymethyl)-11,12-bis-O-(phenylmethyl)-1,3-O-[(R)-phenylmethylene]- (9CI) (CA INDEX NAME)

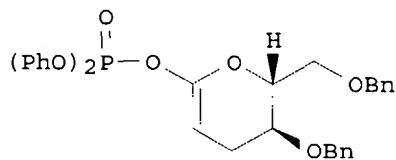
Absolute stereochemistry. Rotation (+).



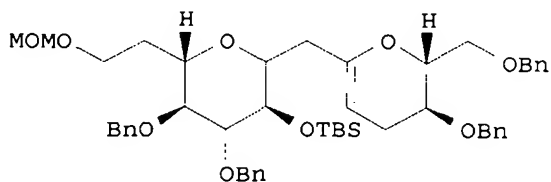
GI



I



II



III

AB Title compds., which are intermediates for (large-membered) cyclic polyethers, e.g. ciguatoxin 3C, are **prepd.** by cross-coupling of alkylboranes with cyclic enol phosphates in the presence of Pd(0) compd. having phosphine ligands as catalysts in basic aq. solns. Thus, exo-olefin I was treated with 9-BBN at 60.degree. in THF and treated with NaHCO<sub>3</sub>, Pd(PPh<sub>3</sub>)<sub>4</sub>, and cyclic enol phosphate II at 50.degree. for 20 h in DMF to give 98% cyclic polyether III.



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L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:279190 CAPLUS

DOCUMENT NUMBER: 135:76718

TITLE: Synthetic studies on a marine polyether toxin,  
gambierol: stereoselective **synthesis** of the  
EFGH ring system via B-alkyl Suzuki coupling

AUTHOR(S): Fuwa, H.; Sasaki, M.; Tachibana, K.

CORPORATE SOURCE: Graduate School of Science, Department of Chemistry,  
Japan Science and Technology Corporation (JST), CREST,  
The University of Tokyo, Bunkyo-ku, Tokyo, 113-0033,  
Japan

SOURCE: Tetrahedron (2001), 57(15), 3019-3033

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:76718

IT 315203-88-4P

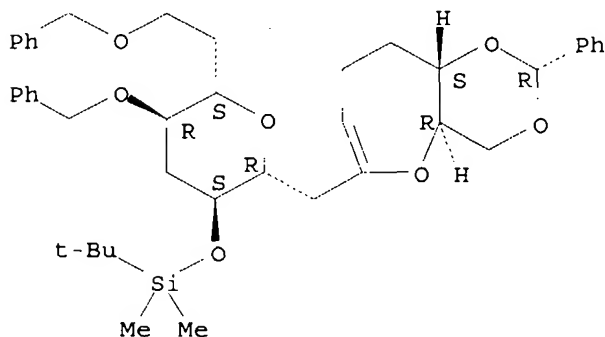
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(synthetic studies on a marine polyether toxin, gambierol,  
stereoselective **synthesis** of EFGH ring system via B-alkyl  
Suzuki coupling)

RN 315203-88-4 CAPLUS

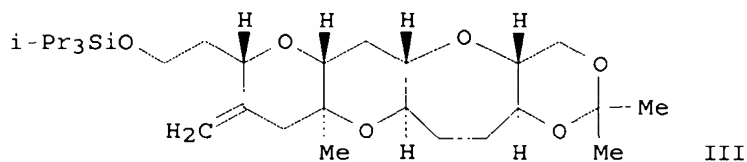
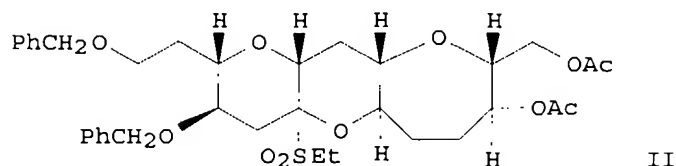
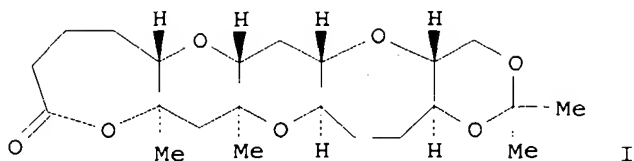
CN Silane, (1,1-dimethylethyl)dimethyl[[[(2R,3S,5R,6S)-tetrahydro-5-  
(phenylmethoxy)-6-[2-(phenylmethoxy)ethyl]-2-[[[(2R,4aR,9aS)-4a,8,9,9a-  
tetrahydro-2-phenyl-4H-1,3-dioxino[5,4-b]oxepin-6-yl]methyl]-2H-pyran-3-  
yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI

10/049,823



AB A synthetic route to the EFGH ring system I of gambierol, a marine polyether toxin isolated from the dinoflagellate *Gambierdiscus toxicus*, has been developed. The present **synthesis** features convergent coupling of the F and H rings followed by ring-closure of the G ring based on the B-alkyl Suzuki reaction of lactone-derived enol phosphates. An angular Me group at C23 was stereoselectively introduced by treatment of sulfone II with trimethylaluminum. Installation of a tertiary alc. at C21 was accomplished through stereoselective dihydroxylation of exo-methylene III followed by selective formation of the primary p-toluenesulfonate and treatment of the resultant monotosylate with lithium aluminum hydride. Finally, formation of the E ring as a lactone form completed the **synthesis** of I.

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:833976 CAPLUS

DOCUMENT NUMBER: 134:71431

TITLE: Synthetic studies on a marine polyether toxin, gambierol: stereoselective **synthesis** of the FGH ring system via B-alkyl Suzuki coupling

AUTHOR(S): Fuwa, Haruhiko; Sasaki, Makoto; Tachibana, Kazuo  
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, The University of Tokyo, Japan Science and Technology Corporation (JST), Tokyo, 113-0033, Japan

SOURCE: Tetrahedron Letters (2000), 41(43), 8371-8375  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:71431

IT 315203-88-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

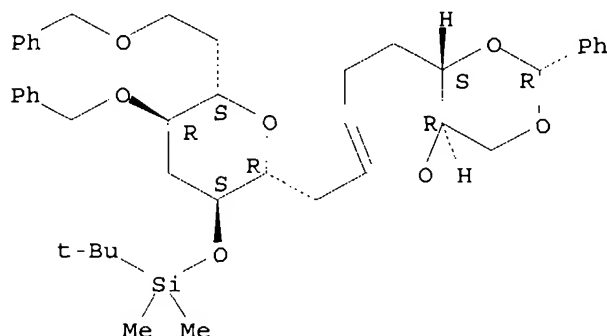
10/049,823

(stereoselective **prepn.** of the gambierol FGH ring system via  
B-alkyl Suzuki coupling)

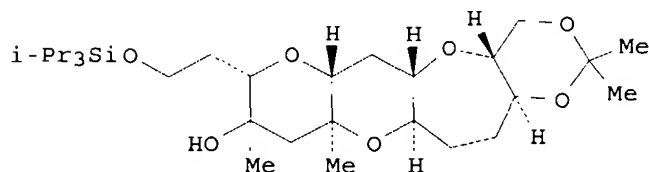
RN 315203-88-4 CAPLUS

CN Silane, (1,1-dimethylethyl)dimethyl[[[(2R,3S,5R,6S)-tetrahydro-5-(phenylmethoxy)-6-[2-(phenylmethoxy)ethyl]-2-[[[(2R,4aR,9aS)-4a,8,9,9a-tetrahydro-2-phenyl-4H-1,3-dioxino[5,4-b]oxepin-6-yl]methyl]-2H-pyran-3-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI



I

AB A synthetic route to the FGH ring system of gambierol, a marine polyether toxin isolated from the dinoflagellate Gambierdiscus toxicus, has been developed. The present **synthesis** features B-alkyl Suzuki coupling of the F and H rings, followed by ring-closure of the G ring and stereoselective installation of 1,3-diaxial Me groups at C21 and C23 to yield I in 75% yield.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:580096 CAPLUS

DOCUMENT NUMBER: 131:351146

TITLE: A General Method for Convergent **Synthesis** of Polycyclic Ethers Based on Suzuki Cross-Coupling: Concise **Synthesis** of the ABCD Ring System of Ciguatoxin

AUTHOR(S): Sasaki, Makoto; Fuwa, Haruhiko; Ishikawa, Makoto; Tachibana, Kazuo

CORPORATE SOURCE: Department of Chemistry School of Science, The

10/049,823

University of Tokyo CREST Japan Science and Technology  
Corporation (JST), Hongo Bunkyo-ku Tokyo, 113-0033,  
Japan

SOURCE: Organic Letters (1999), 1(7), 1075-1077

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

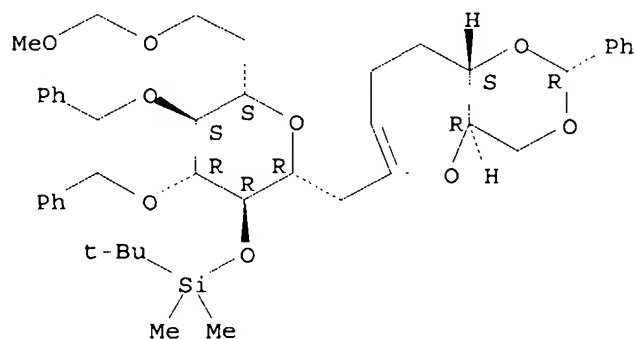
IT 250226-82-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(**synthesis** of the ABCD ring system of ciguatoxin via Suzuki  
cross-coupling)

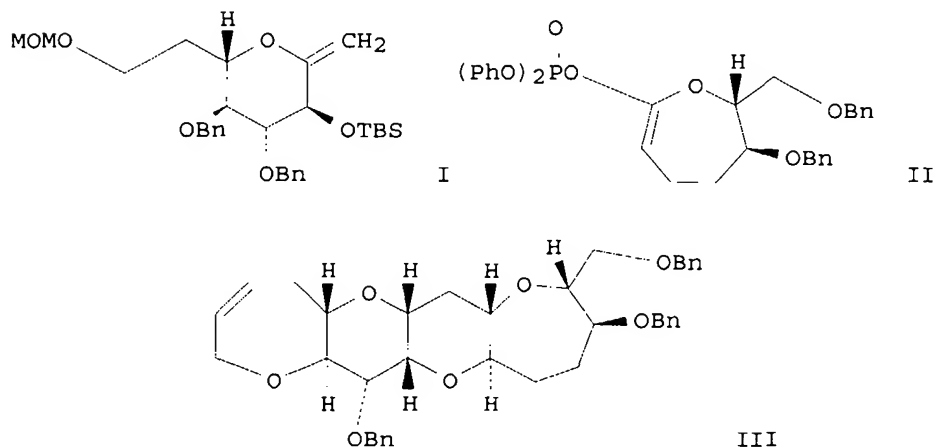
RN 250226-82-5 CAPLUS

CN L-arabino-L-allo-Pentadec-6-enitol, 2,7:9,13-dianhydro-4,5,6,8,14-  
pentadeoxy-10-O-[(1,1-dimethylethyl)dimethylsilyl]-15-O-(methoxymethyl)-  
11,12-bis-O-(phenylmethyl)-1,3-O-[(R)-phenylmethylene]- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry. Rotation (+).



GI



10/049,823

AB A general method for convergent assembly of polyether structure has been developed based on palladium(0)-mediated Suzuki cross-coupling reaction of alkylboranes (I) with cyclic ketene acetal phosphates (II). The present method allowed for coupling of medium-sized ether rings and thus a concise **synthesis** of the ABCD ring system (III) of ciguatoxins has been achieved.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
38.80	187.16

FULL ESTIMATED COST

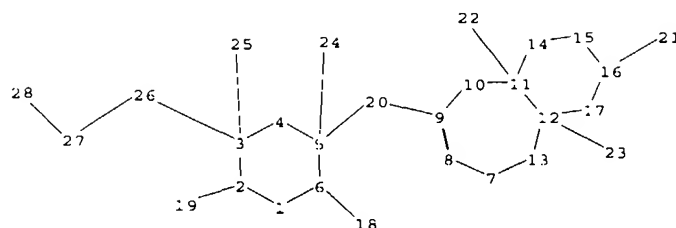
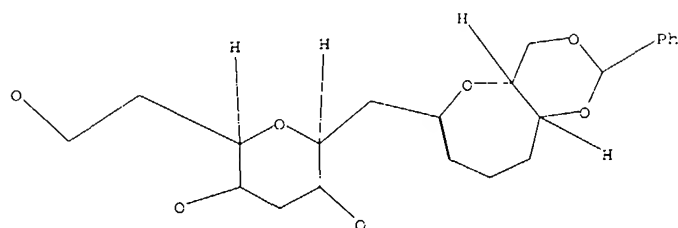
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-3.91	-3.91

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 14:20:52 ON 23 MAY 2003

C:\STNEXP4\QUERIES\10049823.str



chain nodes :

18 19 20 21 22 23 24 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds :

2-19 3-25 3-26 5-20 5-24 6-18 9-20 11-22 12-23 16-21 26-27 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-13 8-9 9-10 10-11 11-12 11-14 12-13 12-17  
14-15 15-16 16-17

exact/norm bonds :

2-19 6-18 27-28

exact bonds :

1-2 1-6 2-3 3-4 3-25 3-26 4-5 5-6 5-20 5-24 7-8 7-13 8-9 9-10 9-20 10-11  
11-12 11-14 11-22 12-13 12-17 12-23 14-15 15-16 16-17 16-21 26-27

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS  
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS